CONTENTS

Investigations of the anaesthetic activity of nitrous oxide by quantum-chemical calculations
J. Sadlej and M. Siciński (Warsaw, Poland) 1

Paramagnetic probes for molecular interactions. Part 4. UHF open-shell SCF study of the interaction of lithium cation with dimethylnitroxide radical
K. Miąskiewicz and W. Kolodziejski (Warsaw, Poland) 15

Ab initio and INDO SCF MO study of monosubstituted hydrazyl radicals
P. Smith and W.H. Donovan (Durham, NC, U.S.A.) 21

A study of the electronic structure and catalytic properties of the Keggin unit $(PMo_{12}O_{40})^{3-}$
S.X. Xiao (Chengdu, China), J. Ji (Dalian, China), T.L. Chen (Chengdu, China), X.T. Cai (Dalian, China) and G.S. Yan (Chengdu, China) 33

A theoretical potential for the puckering of dibenzo-*p*-dioxin
T. Schaefer and R. Sebastian (Winnipeg, Man, Canada) 41

Investigation of heteroaromatic nucleophilic substitution reaction
K.J. Szabó and J. Császár (Budapest, Hungary) 45

Molecular structure and vibrational treatment of dimethyl sulphide and ethyl methyl sulphide in complexes with HCl: a theoretical study
M. Oshaku (Hiroshima, Japan) 57

Rotational barriers adjacent to the C=N double bond in methyl and ethylimines
A. Cossé-Barbi, A.K. Battacharjee, J.-P. Doucet and J.-E. Dubois (Paris, France) 67

Rotational potential energy functions in ethylchlorosilane, (chloromethyl)methylsilane and (chloromethyl)chlorosilane: MM2, MNDO and ab initio calculations
S.G. Cho (Baton Rouge, LA, U.S.A.), F.K. Cartledge and R.J. Unwalla (Research Triangle Park, NC, U.S.A.) 79

The structure of the CH_2O–NH_3 system. Part I. Study of configurations
C. Kozmutza and Zs. Ozoróczy (Budapest, Hungary) and E. Kapuy (Szeged, Hungary) 101

Conformational analysis of an O $(AB)_4$ model for moieties with $S_4(\bar{4})$ symmetry
F.H. Cano, J. Fayos and C. Foces-Foces (Madrid, Spain) 111

Alkyl and acyl substituent effects on nitrenium ion stabilities: ab initio molecular orbital calculations
G.P. Ford and P.S. Herman (Dallas, TX, U.S.A.) 121

1,3-Diphosphabicyclo[1.1.1]pentane dication: theoretical evidence for an inverted phosphorus atom
S.M. Bachrach (DeKalb, IL, U.S.A.) 131

An ab initio study of the conformation and intramolecular proton transfer in the enol form of acetylacetone
M.A. Rios and J. Rodríguez (Galicia, Spain) 137

Electronic and vibrational properties of $ONNO_2$ and ONNSO
S.A. Maluendes, A.H. Jubert and E.A. Castro (La Plata, Argentina) 145

Mechanical and electrical anharmonicities in the hydrogen cyanide hydrogen-bonded clusters
W.B. De Almeida and A. Hinchliffe (Manchester, Gt. Britain) 153

Energy hypersurface for HCN dimer: problems in choosing the configuration space **R**
W.B. De Almeida and A. Hinchliffe (Manchester, Gt. Britain) 171

Ab initio charge distributions in half-cage compounds
P.R. Seidl, K.Z. Leal, J. Walkimar de M. Carneiro (Rio de Janeiro, Brazil), J.G.R. Tostes (Niterói, Brazil), C.A. Taft (Rio de Janeiro, Brazil), B.L. Hammond and W.A. Lester, Jr. (Berkeley, CA, U.S.A.) 182

The vinylcyclopropane rearrangement: an AM1 study
J.J. Quirante, F. Enriquez (Malaga, Spain) and J.M. Hernando (Valladolid, Spain) 193

Study of the interconversion of the isomers of 14-annulene by the AM1 method
J.M. Hernando (Valladolid, Spain), J.J. Quirante and F. Enriquez (Malaga, Spain) 201

Ab initio studies of structural features not easily amenable to experiment. Part 67. The 4-21G optimized structure of a novel cage dimer, $C_{22}H_{24}$ and comparison with its crystal structure
K. Siam (Pittsburg, KS, U.S.A.), C. van Alsenoy (Wilrijk, Belgium), K. Wolinski, L. Schäfer (Fayetteville, AR, U.S.A.), A.P. Marchand, P.-W. Jin and M.N. Deshpande (Denton, TX, U.S.A.) 209
A gradient ab initio study of the geometrical trends of 1,2-dioxocyclopentane and other cyclic peroxides
L. Carballeira, R.A. Mosquera and M.A. Ríos (Galicia, Spain) 219
A model for the elementary prediction of the angular geometries of van der Waals dimers
V. Magnasco, C. Costa and G. Figari (Genoa, Italy) 229
Ab initio study of the disulphide bond. Part 2. The change in atomic distance between sulphur atoms on the reduction of disulphide to dithiol
M. Honda and M. Tajima (Saitama, Japan) 247
An appraisal of solvation effects on chemical functional groups: the amidic and the esteric linkages
G. Alagona, C. Ghio (Pisa, Italy), J. Igual (Tarragona, Spain) and J. Tomasi (Pisa, Italy) 253
Ab initio study of the electronic structures of carbonyl oxides
C. Yang and Y.-L. Wang (Suzhou, China) 285
Ab initio calculations of structural features not easily amenable to experiment. Part 68. Structural trends in some substituted nitriles and acetylenes
K. Siam (Pittsburg, KS, U.S.A.), M. Dakkouri (Ulm, F.R.G.), J.D. Ewbank and L. Schäfer (Fayetteville, AR, U.S.A.) 291
Conformation of cyclodipeptides. Factor analysis: a convenient tool for simplifying conformational studies of condensed poly-ring systems: prolyl-type cyclopeptides
St. Oldziej, P. Dokurno, B. Liberek, A.S. Kolodziejczyk, J. Ciarkowski (Gdańsk, Poland) and M. Gdaniec (Poznań, Poland) 301
Non-empirical cluster-model study of the relaxation of (111) surfaces of C, Si, Ge
V. Barone (Naples, Italy), C. Minichino (Potenza, Italy), N. Russo, M. Toscano (Cosenza, Italy), F. Illas and J. Rubio (Barcelona, Spain) 325
Ab initio investigations of the hydrolysis of the carbamate bond
M. Remko (Bratislava, Czechoslovakia) and S. Scheiner (Carbondale, IL, U.S.A.) 331
A theoretical study of conformations and rotational barriers in dihydroxybenzenes
C. Puebla and T.-K. Ha (Zürich, Switzerland) 337
The influence of water on substituent field effects
J.-F. Cai and R.D. Topsom (Bundoora, Australia) 353
Ab initio studies of structural features not easily amenable to experiment. Part 69. Conformational analysis and structural study of cysteine
L. Schäfer (Fayetteville, AR, U.S.A.), K. Siam (Pittsburg, KS, U.S.A.), V.J. Klimkowski, J.D. Ewbank (Fayetteville, AR, U.S.A.) and C. van Alsenoy (Wilrijk, Belgium) 361
Theory of phase factors for a one-body potential of arbitrary symmetry
P.M. Kozlowski and N.H. March (Oxford, Gt. Britain) 373
Theoretical investigation of lipid peroxidation mechanism
G. Saba (Cagliari, Italy), P. Scano, P.A. Sedda and C. Thomson (St. Andrews, Gt. Britain) .. 379
Topomerization, tautomerization and deprotonation of $S_2H_3^{\oplus}$
M. Loos, J.-L. Rivail (Nancy, France) and I. Csizmadia (Toronto, Ont., Canada) 389

Book review 397

Announcements 399

Author index 403

Subject index 405